AN ANALYSIS OF THE EFFECT OF GHOST FORCE OSCILLATION ON QUASICONTINUUM ERROR

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Abstract. The atomistic to continuum interface for quasicontinuum energies exhibits nonzero forces under uniform strain that have been called ghost forces. In this paper, we prove for a linearization of a one-dimensional quasicontinuum energy around a uniform strain that the effect of the ghost forces on the displacement nearly cancels and has a small effect on the error away from the interface. We give optimal order error estimates that show that the quasicontinuum displacement converges to the atomistic displacement at the rate $\mathrm{O}(h)$ in the discrete ℓ^∞ and $w^{1,1}$ norms where h is the interatomic spacing. We also give a proof that the error in the displacement gradient decays away from the interface to $\mathrm{O}(h)$ at distance $\mathrm{O}(h|\log h|)$ in the atomistic region and distance $\mathrm{O}(h)$ in the continuum region. E, Ming, and Yang previously gave a counterexample to convergence in the $w^{1,\infty}$ norm for a harmonic interatomic potential. Our work gives an explicit and simplified form for the decay of the effect of the atomistic to continuum coupling error in terms of a general underlying interatomic potential and gives the estimates described above in the discrete ℓ^∞ and $w^{1,p}$ norms.

1. Introduction

The quasicontinuum method (QC) reduces the computational complexity of atomistic simulations by replacing smoothly varying regions of the material with a continuum approximation derived from the atomistic model [5–9,11–15,17,18,21,23,25]. This is extremely effective in simulations involving defects, which have singularities in the deformation gradient. In such simulations, a few localized regions require the accuracy and high computational expense of atomistic scale resolution, but the rest of the material has a slowly varying deformation gradient which can be more efficiently computed using the continuum approximation without loss of the desired accuracy. Adaptive algorithms have been developed for QC to determine which regions require the accuracy of atomistic modeling and how to coarsen the finite element mesh in the continuum region [1–3, 16–18, 20]. The atoms retained in the atomistic region and the atoms at nodes of the piecewise linear finite element mesh in the continuum region are collectively denoted as *representative atoms*.

Recent years have seen the development of many QC approximations that differ in how they compute interactions among the representative atoms. In the following, we concern ourselves with the original energy-based quasicontinuum (QCE) approximation [15, 25], but the phenomena that we analyze occur in all other quasicontinuum approximations, as well as in other multiphysics coupling methods [8]. In QCE, a total energy is created by summing energy contributions from each representative atom in the atomistic region and from each element in the continuum region, where the volume of the elements in the atomistic to continuum interface is modified to exactly

Date: November 26, 2008.

2000 *Mathematics Subject Classification.* 65Z05,70C20.

This work was supported in part by DMS-0757355, DMS-0811039, the Institute for Mathematics and Its Applications, the University of Minnesota Supercomputing Institute, and the University of Minnesota Doctoral Dissertation Fellowship. This work is also based on work supported by the Department of Energy under Award Number DE-FG02-05ER25706.

conserve mass. This construction was chosen so that for any uniform strain the QCE energy, the continuum energy, and the atomistic energy are identical. (As discussed later, this conservation property for the QCE approximation is not sufficient to prevent the existence of nonzero forces at the atomistic to continuum interface for uniform strain.) The representative atoms then interact via forces defined by the total energy. This makes for a simple and versatile method that can treat complicated geometries and can be used with adaptive algorithms that modify the mesh and atomistic regions during a quasi-static process. Other atomistic to continuum approaches have been proposed, for example, that utilize overlapping or blended domains [4, 19].

One drawback of the energy-based quasicontinuum approximation that has received much attention is the fact that at the atomistic to continuum interface the balance of force equations do not give a consistent scheme [22]. As explained in Section 2, the equilibrium equations in the interior of both the atomistic region and the continuum region give consistent finite difference schemes for the continuum limit, whereas the QC equilibrium equations near the interface are not consistent with the continuum limit. This is most easily seen by considering a uniform strain, which will be assigned identically zero elastic forces by any consistent scheme. (Ensuring that a given scheme assigns zero forces for uniform strain has been known as the "patch test" in the theory of finite elements [24].) The nonzero residual forces present in QCE for uniform strain have been called "ghost forces" [7, 22].

In this paper, we give optimal order error estimates for the effect of the inconsistency on the displacement and displacement gradient for a linearization of a one-dimensional atomistic energy and its quasicontinuum approximation. We consider the linearization of general interatomic potentials which are concave near second-neighbor interatomic distances. This property guarantees that the interfacial error due to the Cauchy-Born approximation with a second-neighbor cut-off is positive [7, p. 117] and that the quasicontinuum error is not oscillatory in the atomistic region (see Section 3). Similar optimal order error estimates have been given by E, Ming, and Yang [10] for a harmonic interatomic potential.

We begin by linearizing a one-dimensional atomistic energy, its local quasicontinuum approximation (which we will call the continuum energy), and its quasicontinuum approximation about a uniform strain for a second-neighbor atomistic energy. We will show in Section 2 that the three systems of equilibrium equations are then

$$\begin{aligned} L^{a,h}\mathbf{u}_a &= \mathbf{f}, && \text{(atomistic)} \\ L^{c,h}\mathbf{u}_c &= \mathbf{f}, && \text{(continuum)} \\ L^{qc,h}\mathbf{u}_{qc} - \mathbf{g} &= \mathbf{f}, && \text{(quasicontinuum)} \end{aligned}$$

where $\mathbf{f}$ is an external loading, L and $\mathbf{u}$ are the linearized operator and corresponding displacement for each scheme, $\mathbf{g}$ is non-zero only in the atomistic to continuum interface, and h is the interatomic spacing. The term $\mathbf{g}$ in the quasicontinuum equilibrium equations is due to the unbalanced second-neighbor interactions in the interface (2.13) and for uniform stretches is precisely the ghost force described in [7, 15, 22].

Formally, the error decomposes as

$$\mathbf{u}_a - \mathbf{u}_{qc} = ((L^{a,h})^{-1} - (L^{qc,h})^{-1})\mathbf{f} - (L^{qc,h})^{-1}\mathbf{g}.$$

(The operators are all translation invariant, so they only have solutions up to the choice of an additive constant.) In this paper, we focus on the second term, $(L^{qc})^{-1}\mathbf{g}$, which is the error due to the inconsistency at the interface. To do so, we consider the case of no external field, $\mathbf{f} = \mathbf{0}$, which will make $\mathbf{u}_a = \mathbf{0}$. For most applications of the quasicontinuum method, the only external field is

due to loads that are applied on the boundary of the material, far from the atomistic to continuum interface.

We showed in [7] that the ghost forces are oscillatory and sum to zero. In this paper, we prove that the error in the displacement gradient is O(1) at the interface and decays away from the interface to O(h) at distance O($h|\log h|$) in the atomistic region and distance O(h) in the continuum region. As noted above, similar results have been given in [10] for a harmonic interatomic potential with $\mathbf{f} \neq \mathbf{0}$ and Dirichlet boundary conditions. Here, we present a simplified approach starting from a linearization of a quasicontinuum approximation with a concave second-neighbor interaction. We explicitly give the form of the solution and analyze the solution in discrete l^∞ and $w^{1,p}$ norms. We show that the quasicontinuum displacement converges to the atomistic displacement at the rate O(h) in the discrete l^∞ and $w^{1,1}$ norms where h is the interatomic spacing.

In Section 2, we describe the energy-based quasicontinuum approximation (QCE) and set up the analysis. In Section 3, we prove Theorem 3.1 for the quasicontinuum energy that gives an optimal order, O(h) error estimate in the l^∞ norm and a O($h^{1/p}$) error estimate in the $w^{1,p}$ norm for $1 \leq p < \infty$. Note that for simplicity the models and analysis are presented for the case where no degrees of freedom have been removed in the continuum region, but we explain in Remark 3.1 that identical results hold when the continuum region is coarsened. We present numerical computations in Figure 1 that clearly show that the error is localized in the atomistic to continuum interface.

2. One-Dimensional, Linear Quasicontinuum Approximation

We consider an infinite one-dimensional chain of atoms with periodicity $2F$ in the deformed configuration. Let y_j denote the atomic positions for $-\infty < j < \infty$, where there are $2N$ atoms in each period. Let $h = 1/N$ and let

$$u_j := y_j - Fhj$$

denote the displacement from the average interatomic spacing, Fh. In the following, we analyze the behavior of the quasicontinuum method as the atomistic chain approaches the continuum limit with F fixed and $N \to \infty$.

The atomistic energy for a period of the chain is

$$\mathcal{E}^{tot,h}(\mathbf{y}) := h \sum_{j=-N+1}^{N} \left[\phi\left(\frac{y_{j+1} - y_j}{h}\right) + \phi\left(\frac{y_{j+2} - y_j}{h}\right) - f_j y_j \right], \tag{2.1}$$

where $\phi(r)$ is a two-body interatomic potential (for example, the Lennard-Jones potential $\phi(r) = 1/r^{12} - 2/r^6$) and $\mathbf{f} = (f_{-N+1}, \ldots, f_N)$ are external forces applied as dead loads on the atoms. The periodic conditions

$$y_{j+2N} = y_j + 2F \qquad \text{or} \qquad u_{j+2N} = u_j$$

allow $\mathcal{E}^{tot,h}$ to be written in terms of $\mathbf{y} := (y_{-N+1}, \ldots, y_N)$. We assume that $\sum_{-N+1}^{N} f_j = 0$, otherwise there are no energy minimizing solutions since the elastic energy is translation invariant. In the following, we discuss the existence and uniqueness of solutions to each of the models we encounter. We note that the energy per bond in (2.1) has been scaled like $h\phi(r/h)$. This scaling implies that if we let $y_j = y(j/N)$ and $f_j = f(j/N)$ for $j = -N+1, \ldots, N$ where $y \in C^1([-1,1])$ and $f \in C([-1,1])$, then as $N \to \infty$ and F is held fixed, the energy of a period (2.1) converges to

$$\int_{-1}^{1} \phi(y'(x)) + \phi(2y'(x)) - f(x)y(x)\,\mathrm{d}x.$$

We expand first neighbor terms around F, giving

$$\begin{aligned}\phi\left(\frac{y_{j+1}-y_j}{h}\right) &= \phi\left(F+\frac{u_{j+1}-u_j}{h}\right)\\ &= \phi(F)+\phi'(F)\,\frac{u_{j+1}-u_j}{h}+\tfrac{1}{2}\phi''(F)\left(\frac{u_{j+1}-u_j}{h}\right)^2+O\left(\left|\frac{u_{j+1}-u_j}{h}\right|^3\right),\end{aligned}$$

and the second neighbor terms around $2F$, giving

$$\begin{aligned}\phi\left(\frac{y_{j+2}-y_j}{h}\right) &= \phi\left(2F+\frac{u_{j+2}-u_j}{h}\right)\\ &= \phi(2F)+\phi'(2F)\,\frac{u_{j+2}-u_j}{h}+\tfrac{1}{2}\phi''(2F)\left(\frac{u_{j+2}-u_j}{h}\right)^2+O\left(\left|\frac{u_{j+2}-u_j}{h}\right|^3\right).\end{aligned}$$

2.1. **Atomistic Model.** The linearized atomistic energy is then given by

$$\begin{aligned}\mathcal{E}^{a,h}(\mathbf{u}) := h\sum_{j=-N+1}^{N}\Bigg[&\phi'_F\,\frac{u_{j+1}-u_j}{h}+\tfrac{1}{2}\phi''_F\left(\frac{u_{j+1}-u_j}{h}\right)^2\\ &+\phi'_{2F}\,\frac{u_{j+2}-u_j}{h}+\tfrac{1}{2}\phi''_{2F}\left(\frac{u_{j+2}-u_j}{h}\right)^2-f_ju_j\Bigg],\end{aligned}\tag{2.2}$$

where $\phi'_F := \phi'(F), \phi''_F := \phi''(F), \phi'_{2F} := \phi'(2F), \phi''_{2F} := \phi''(2F)$, and $\mathbf{u} := (u_{-N+1},\dots,u_N)$. Note that here and in the following, we neglect the additive constant $\phi(F)+\phi(2F)-h\sum_{j=-N+1}^{N} f_jFhj$ in the linearized energy. We assume that $\phi \in C^2([r_0,\infty))$ for some r_0 such that $0<r_0<F$, and

$$\phi''_F > 0 \text{ and } \phi''_{2F} < 0.\tag{2.3}$$

This holds true for the Lennard-Jones potential for Fh below the load limit, unless the chain is extremely compressed (less than 60% of the equilibrium length). The property $\phi''_{2F}<0$ ensures that the quasicontinuum error is not oscillatory in the atomistic region (see Section 3).

We furthermore assume that

$$\phi''_F + 5\phi''_{2F} > 0,\tag{2.4}$$

which will be sufficient to give solutions to the QC equilibrium equations under the assumption of no resultant external forces (see Lemma 2.1). In contrast, the weaker assumption $\phi''_F+4\phi''_{2F}>0$ is sufficient for the fully atomistic or fully continuum approximation. The equilibrium equations, $\frac{1}{h}\frac{\partial\mathcal{E}^{a,h}}{\partial u_j}(\mathbf{u})=0$, for the atomistic model (2.2) are

$$\begin{aligned}(L^{a,h}\mathbf{u})_j = \frac{-\phi''_{2F}u_{j+2}-\phi''_Fu_{j+1}+2(\phi''_F+\phi''_{2F})u_j-\phi''_Fu_{j-1}-\phi''_{2F}u_{j-2}}{h^2} &= f_j,\\ u_{j+2N} &= u_j,\end{aligned}\tag{2.5}$$

for $-\infty<j<\infty$. Note that scaling by $\frac{1}{h}$ makes this a consistent approximation of the boundary value problem

$$\begin{aligned}-(\phi''_F+4\phi''_{2F})u''(x) &= f \qquad \text{for } -\infty<x<\infty,\\ u(x+2) &= u(x) \qquad \text{for } -\infty<x<\infty.\end{aligned}\tag{2.6}$$

The linearized atomistic energy (2.2) has a unique minimum (up to a constant) if $\phi''_F+4\phi''_{2F}>0$, provided that $\sum_{j=N-1}^{N} f_j = 0$. Standard ODE results show that (2.6) has a unique solution (up to a constant) provided that $\int_{-1}^{1} f(x)\,\mathrm{d}x = 0$.

Remark 2.1. For the atomistic energy (2.2), the linear terms sum to zero by the periodicity of the displacement, since

$$h\sum_{j=-N+1}^{N}\left[\phi_F'\,\frac{u_{j+1}-u_j}{h}+\phi_{2F}'\,\frac{u_{j+2}-u_j}{h}\right]$$
$$=\phi_F'\left[u_{N+1}-u_{-N+1}\right]+\phi_{2F}'\left[u_{N+2}+u_{N+1}-u_{-N+2}-u_{-N+1}\right]=0.$$

However, we keep these terms in the model since they do not sum to zero when the atomistic model is coupled to the continuum approximation in the quasicontinuum energy. The resulting terms give a more accurate representation of what happens in the non-linear quasicontinuum model.

2.2. **Continuum Approximation.** The continuum approximation splits the chain into linear finite elements with nodes given by the representative atoms, which we recall are a subset of the atoms in the chain. The energy of the chain is the sum of element energies which depend only on the element's deformation gradient, the linear deformation that interpolates its nodal positions. The energy of an element is then computed by applying the element's deformation gradient to the reference lattice, computing the energy per atom using the atomistic model, and multiplying by the number of atoms in the element (where the boundary atoms are shared equally between neighboring elements). If the continuum approximation is not coarsened (every atom is a representative atom), then the continuum energy is given by

$$\mathcal{E}^{c,h}(\mathbf{u}):=h\sum_{j=-N+1}^{N}\left[(\phi_F'+2\phi_{2F}')\left(\frac{u_{j+1}-u_j}{h}\right)+\tfrac{1}{2}(\phi_F''+4\phi_{2F}'')\left(\frac{u_{j+1}-u_j}{h}\right)^2-f_ju_j\right]. \quad (2.7)$$

See [7] for a derivation of the continuum energy and a discussion of the error terms at the element boundaries. For $j\in\{-N+1,\dots,N\}$, the equilibrium equations for the continuum approximation are

$$(L^{c,h}\mathbf{u})_j=(\phi_F''+4\phi_{2F}'')\left[\frac{-u_{j+1}+2u_j-u_{j-1}}{h^2}\right]=f_j, \quad (2.8)$$

which is also a consistent approximation for the boundary value problem (2.6). It is easy to see that the continuum energy (2.7) has a unique minimum (up to a constant) if $\phi_F''+4\phi_{2F}''>0$, provided that $\sum_{j=N-1}^{N}f_j=0$. The quasicontinuum method inherently supports coarsening, but we neglect it here since in one dimension this only changes the scaling of equilibrium equations.

2.3. **Splitting the Energy.** We can split the atomistic energy and the continuum energy into per-atom contributions so that

$$\mathcal{E}^{a,h}(\mathbf{u})=h\sum_{j=-N+1}^{N}\left[\mathcal{E}_j^{a,h}(\mathbf{u})-f_ju_j\right]\quad\text{and}\quad\mathcal{E}^{c,h}(\mathbf{u})=h\sum_{j=-N+1}^{N}\left[\mathcal{E}_j^{c,h}(\mathbf{u})-f_ju_j\right].$$

There are many possible ways to define the per-atom contributions, and we do this in such a way that these contributions are linearizations of the ones in the fully nonlinear case presented in [7,25].

In this case, we split the energy of each bond to obtain

$$\begin{aligned}\mathcal{E}_j^{a,h}(\mathbf{u}) := \frac{1}{2}\Bigg[&\phi_F' \frac{u_{j+1}-u_j}{h} + \tfrac{1}{2}\phi_F''\left(\frac{u_{j+1}-u_j}{h}\right)^2 \\ &+ \phi_{2F}' \frac{u_{j+2}-u_j}{h} + \tfrac{1}{2}\phi_{2F}''\left(\frac{u_{j+2}-u_j}{h}\right)^2\Bigg] \\ +\frac{1}{2}\Bigg[&\phi_F' \frac{u_j-u_{j-1}}{h} + \tfrac{1}{2}\phi_F''\left(\frac{u_j-u_{j-1}}{h}\right)^2 \\ &+ \phi_{2F}' \frac{u_j-u_{j-2}}{h} + \tfrac{1}{2}\phi_{2F}''\left(\frac{u_j-u_{j-2}}{h}\right)^2\Bigg],\end{aligned} \tag{2.9}$$

and

$$\begin{aligned}\mathcal{E}_j^{c,h}(\mathbf{u}) := \frac{1}{2}&\left[(\phi_F' + 2\phi_{2F}')\left(\frac{u_{j+1}-u_j}{h}\right) + \tfrac{1}{2}(\phi_F'' + 4\phi_{2F}'')\left(\frac{u_{j+1}-u_j}{h}\right)^2\right] \\ &+ \frac{1}{2}\left[(\phi_F' + 2\phi_{2F}')\left(\frac{u_j-u_{j-1}}{h}\right) + \tfrac{1}{2}(\phi_F'' + 4\phi_{2F}'')\left(\frac{u_j-u_{j-1}}{h}\right)^2\right].\end{aligned} \tag{2.10}$$

2.4. **Energy-Based Quasicontinuum Approximation.** The energy-based quasicontinuum approximation partitions the representative atoms into atomistic and continuum representative atoms and assigns to each atom the split energy corresponding to its type (2.9-2.10). We define the nodes $-N+1,\ldots,-K-1$ and $K+1,\ldots,N$ to be continuum and $-K,\ldots,K$ to be atomistic, where we assume that $2 \le K \le N-2$ to ensure well-defined atomistic and continuum regions. The quasicontinuum energy is then

$$\mathcal{E}^{qc,h}(\mathbf{u}) := \sum_{j=-N+1}^{-K-1} \mathcal{E}_j^{c,h}(\mathbf{u}) + \sum_{j=-K}^{K} \mathcal{E}_j^{a,h}(\mathbf{u}) + \sum_{j=K+1}^{N} \mathcal{E}_j^{c,h}(\mathbf{u}) - \sum_{j=-N+1}^{N} f_j u_j. \tag{2.11}$$

Since the energy is quadratic, the equilibrium equations, $\frac{1}{h}\frac{\partial \mathcal{E}^{qc,h}}{\partial u_j}(\mathbf{u}_{qc}) = 0$, take the form

$$L^{qc,h}\mathbf{u}_{qc} - \mathbf{g} = \mathbf{f}. \tag{2.12}$$

For $0 \le j \le N$, the QCE operator is given by

$$(L^{qc,h}\mathbf{u})_j = \phi_F'' \frac{-u_{j+1}+2u_j-u_{j-1}}{h^2} + \begin{cases} 4\phi_{2F}'' \dfrac{-u_{j+2}+2u_j-u_{j-2}}{4h^2}, & 0 \le j \le K-2, \\ 4\phi_{2F}'' \dfrac{-u_{j+2}+2u_j-u_{j-2}}{4h^2} + \dfrac{\phi_{2F}''}{h}\dfrac{u_{j+2}-u_j}{2h}, & j = K-1, \\ 4\phi_{2F}'' \dfrac{-u_{j+2}+2u_j-u_{j-2}}{4h^2} - \dfrac{2\phi_{2F}''}{h}\dfrac{u_{j+1}-u_j}{h} + \dfrac{\phi_{2F}''}{h}\dfrac{u_{j+2}-u_j}{2h}, & j = K, \\ 4\phi_{2F}'' \dfrac{-u_{j+1}+2u_j-u_{j-1}}{h^2} - \dfrac{2\phi_{2F}''}{h}\dfrac{u_j-u_{j-1}}{h} + \dfrac{\phi_{2F}''}{h}\dfrac{u_j-u_{j-2}}{2h}, & j = K+1, \\ 4\phi_{2F}'' \dfrac{-u_{j+1}+2u_j-u_{j-1}}{h^2} + \dfrac{\phi_{2F}''}{h}\dfrac{u_j-u_{j-2}}{2h}, & j = K+2, \\ 4\phi_{2F}'' \dfrac{-u_{j+1}+2u_j-u_{j-1}}{h^2}, & K+3 \le j \le N. \end{cases}$$

Similarly, $\mathbf{g}$ is given by

$$g_j = \begin{cases} 0, & 0 \le j \le K-2, \\ -\frac{1}{2}\phi_{2F}'/h, & j = K-1, \\ \frac{1}{2}\phi_{2F}'/h, & j = K, \\ \frac{1}{2}\phi_{2F}'/h, & j = K+1, \\ -\frac{1}{2}\phi_{2F}'/h, & j = K+2, \\ 0, & K+3 \le j \le N. \end{cases} \tag{2.13}$$

For space reasons, we only list the entries for $0 \le j \le N$. The equations for all other $j \in \mathbb{Z}$ follow from symmetry and periodicity. Due to the symmetry in the definition of the atomistic and continuum regions, we have that $L^{qc,h}_{i,j} = L^{qc,h}_{-i,-j}$ and $g_j = -g_{-j}$ for $-N+1 \le i,j \le 0$. To see this, we define the involution operator $(S\mathbf{u})_j = -u_{-j}$ and observe that $\mathcal{E}^{qc,h}(S\mathbf{u}) = \mathcal{E}^{qc,h}(\mathbf{u})$. It then follows from the chain rule that

$$S^T L^{qc,h} S\mathbf{u} - S^T\mathbf{g} - S^T\mathbf{f} = L^{qc,h}\mathbf{u} - \mathbf{g} - \mathbf{f} \quad \text{for all periodic } \mathbf{u} \text{ and } \mathbf{f}.$$

Since $S^T = S$, we can conclude that

$$SL^{qc,h}S = L^{qc,h} \quad \text{and} \quad Sg = g. \tag{2.14}$$

Note that the expression for $\mathbf{g}$ does not depend on ϕ_F' since the first-neighbor terms identically sum to zero in the energy (2.11). We can now observe that the QCE approximation (2.12) is not consistent with the continuum limit of the atomistic model (2.6).

The linear operator L^{qc} has all uniform translations, $\mathbf{u} = c\mathbf{1} = (c, c, \ldots, c)$, in its nullspace. To see that this is the full nullspace, we consider the factored operator $L^{qc} = D^T E^{qc} D$, where $(D\mathbf{u})_j = \frac{u_{j+1}-u_j}{h}$ and

$$(E^{qc}\mathbf{r})_j = \begin{cases} \phi_{2F}''r_{j-1} + (\phi_F'' + 2\phi_{2F}'')r_j + \phi_{2F}''r_{j+1}, & 0 \le j \le K-2, \\ \phi_{2F}''r_{j-1} + (\phi_F'' + \frac{3}{2}\phi_{2F}'')r_j + \frac{1}{2}\phi_{2F}''r_{j+1}, & j = K-1, \\ \frac{1}{2}\phi_{2F}''r_{j-1} + (\phi_F'' + 3\phi_{2F}'')r_j + \frac{1}{2}\phi_{2F}''r_{j+1}, & j = K, \\ \frac{1}{2}\phi_{2F}''r_{j-1} + (\phi_F'' + \frac{9}{2}\phi_{2F}'')r_j, & j = K+1, \\ (\phi_F'' + 4\phi_{2F}'')r_j, & K+2 \le j \le N. \end{cases}$$

We see that E^{qc} is diagonally dominant provided $\phi_F''+5\phi_{2F}''>0$, hence assumption (2.4) implies E^{qc} is invertible. So we have that the nullspace of L^{qc} is precisely the nullspace of D. Thus, $L^{qc}\mathbf{u}=\mathbf{g}$ has a solution whenever $\sum_{j=-N+1}^{N} f_j=0$, since $\sum_{j=-N+1}^{N} g_j=0$. This solution is unique up to a constant.

We now gather together the existence and uniqueness results stated for the models.

Lemma 2.1. *If $\sum_{j=-N+1}^{N} f_j=0$ and $\phi_F''+4\phi_{2F}''>0$, then the linearized atomistic energy* (2.2) *and continuum approximation* (2.7) *both have a global minimum that is unique up to an additive constant.*

Under the slightly stronger assumption $\phi_F''+5\phi_{2F}''>0$, the quasicontinuum energy (2.11) *has a unique minimizer up to a constant.*

Here, and in the following, we take $\mathbf{f}=\mathbf{0}$, in order to focus on the effect of the ghost force $\mathbf{g}$. Under this assumption, we can conclude that the unique mean zero solution to the QCE equilibrium equations (2.12) is odd. This follows from $S^{-1}=S$ and (2.14) which together imply that $S\mathbf{u}$ is a solution if and only if $\mathbf{u}$ is. Because S preserves the mean zero property, we conclude that $\mathbf{u}_{qc}$ is odd. The unique odd solution to the atomistic equations, $L^{a,h}\mathbf{u}_a=\mathbf{0}$, is $\mathbf{u}_a=\mathbf{0}$. Thus, the QCE equilibrium equations,

$$L^{qc,h}\mathbf{u}_{qc}-\mathbf{g}=\mathbf{0}, \tag{2.15}$$

are also the error equations, and the quasicontinuum solution is the error in approximating $\mathbf{u}_a$.

2.5. **Discrete Sobolev Norms.** The effect of the interface terms on the total error is norm-dependent, so we now employ discrete analogs of Sobolev norms [18]. We define the discrete weak derivative by

$$u_j'=\frac{u_{j+1}-u_j}{h}.$$

For $1\le p<\infty$ the discrete Sobolev norms are given by

$$||u||_{\ell_h^p}=\left(\sum_{j=-N+1}^{N} h|u_j|^p\right)^{1/p},$$
$$||u||_{w_h^{1,p}}=||u||_{\ell_h^p}+\left|\left|u'\right|\right|_{\ell_h^p},$$

and for $p=\infty$ by

$$||u||_{\ell_h^\infty}=\max_{-N+1\le j\le N}|u_j|,$$
$$||u||_{w_h^{1,\infty}}=||u||_{\ell_h^\infty}+\left|\left|u'\right|\right|_{\ell_h^\infty}.$$

The above discrete Sobolev norms are equivalent to the standard Sobolev norms restricted to the continuous, piecewise linear interpolants $u(x)$ satisfying $u(j/N)=u_j$ for $j=-N+1,\dots,N$.

3. Convergence of the Quasicontinuum Solution

We now analyze the quasicontinuum error, $\mathbf{u}_{qc}$. We note that is it theoretically possible to solve (2.15) explicitly for $\mathbf{u}_{qc}$; however, the form of the solution is complicated by the second-neighbor coupling in the atomistic region, so we instead obtain estimates for the decay of the error, $\mathbf{u}_{qc}$, by analyzing a $\mathrm{O}(h^2)$-accurate approximation of the error. Figure 1 shows the results of solving (2.15) numerically for odd solutions, $u_j=-u_{-j}$, with three choices of lattice spacing and two sets of parameters. Note that for both sets of parameters, the magnitude decays linearly with

h, whereas the displacement gradient is O(1) in the atomistic to continuum region. The following argument proves the qualitative error behavior analytically.

3.1. **Form of the Solution.** In the interior of the continuum region the solution is linear, but in the atomistic region $\mathbf{u}_{qc}$ is the sum of a linear solution and exponential solutions. The homogeneous atomistic difference scheme

$$-\phi''_{2F}u_{j+2} - \phi''_F u_{j+1} + (2\phi''_F + 2\phi''_{2F})u_j - \phi''_F u_{j-1} - \phi''_{2F}u_{j-2} = 0 \tag{3.1}$$

has characteristic equation

$$-\phi''_{2F}\Lambda^2 - \phi''_F\Lambda + (2\phi''_F + 2\phi''_{2F}) - \phi''_F\Lambda^{-1} - \phi''_{2F}\Lambda^{-2} = 0,$$

with roots

$$1, 1, \lambda, \frac{1}{\lambda},$$

where

$$\lambda = \frac{(\phi''_F + 2\phi''_{2F}) + \sqrt{(\phi''_F)^2 + 4\phi''_F\phi''_{2F}}}{-2\phi''_{2F}}.$$

Based on the assumptions on ϕ in (2.3) and (2.4), we have that $\lambda > 1$. We note that if ϕ''_{2F} were positive contrary to assumption (2.3), then λ would be negative which would give a damped oscillatory error in the atomistic region. General solutions of the homogeneous atomistic equations (3.1) have the form $u_j = C_1 + C_2hj + C_3\lambda^j + C_4\lambda^{-j}$, but seeking an odd solution reduces this to the form $u_j = C_2hj + C_3(\lambda^j - \lambda^{-j})$.

The odd solution of the quasicontinuum error equations (2.15) is thus of the form

$$(\mathbf{u}_{qc})_j = \begin{cases} m_1hj + \beta\left(\frac{\lambda^j - \lambda^{-j}}{\lambda^K}\right), & 0 \le j \le K, \\ m_2hj - m_2 + \tilde{u}_{K+1}, & j = K+1, \\ m_2hj - m_2, & K+2 \le j \le N, \end{cases}$$

where expressing the unknown u_{K+1} using a perturbation of the linear solution, $\tilde{u}_{K+1}$, simplifies the solution of the equilibrium equations. The four coefficients $m_1,\ m_2, \tilde{u}_{K+1},$ and β can be found by satisfying the four equations in the interface, $j = K-1, \ldots, K+2$. Summing the equilibrium equations across the interface gives

$$\begin{aligned} 0 = \sum_{j=K-1}^{K+2} g_j &= \sum_{j=K-1}^{K+2} (L^{qc,h}\mathbf{u}_{qc})_j \\ &= \phi''_F\,\frac{u_{K-1} - u_{K-2}}{h^2} + 4\phi''_{2F}\,\frac{u_K + u_{K-1} - u_{K-2} - u_{K-3}}{4h^2} \\ &\quad - (\phi''_F + 4\phi''_{2F})\left(\frac{u_{K+3} - u_{K+2}}{h^2}\right) \\ &= (\phi''_F + 4\phi''_{2F})\left(\frac{m_1}{h} - \frac{m_2}{h}\right). \end{aligned}$$

The cancellation of the exponential terms in the final equality holds because

$$\phi''_{2F}(\lambda^K - \lambda^{-K}) + (\phi''_F + \phi''_{2F})(\lambda^{K-1} - \lambda^{-K+1} - \lambda^{K-2} + \lambda^{-K+2}) + \phi''_{2F}(-\lambda^{K-3} + \lambda^{-K+3}) = 0,$$

which can be seen by summing (3.1) with the homogeneous solution $u_j = -\lambda^j$ for $j = -K+2, \ldots, K-2$. Thus $m_1 = m_2$, that is, the slope of the linear part does not change across the

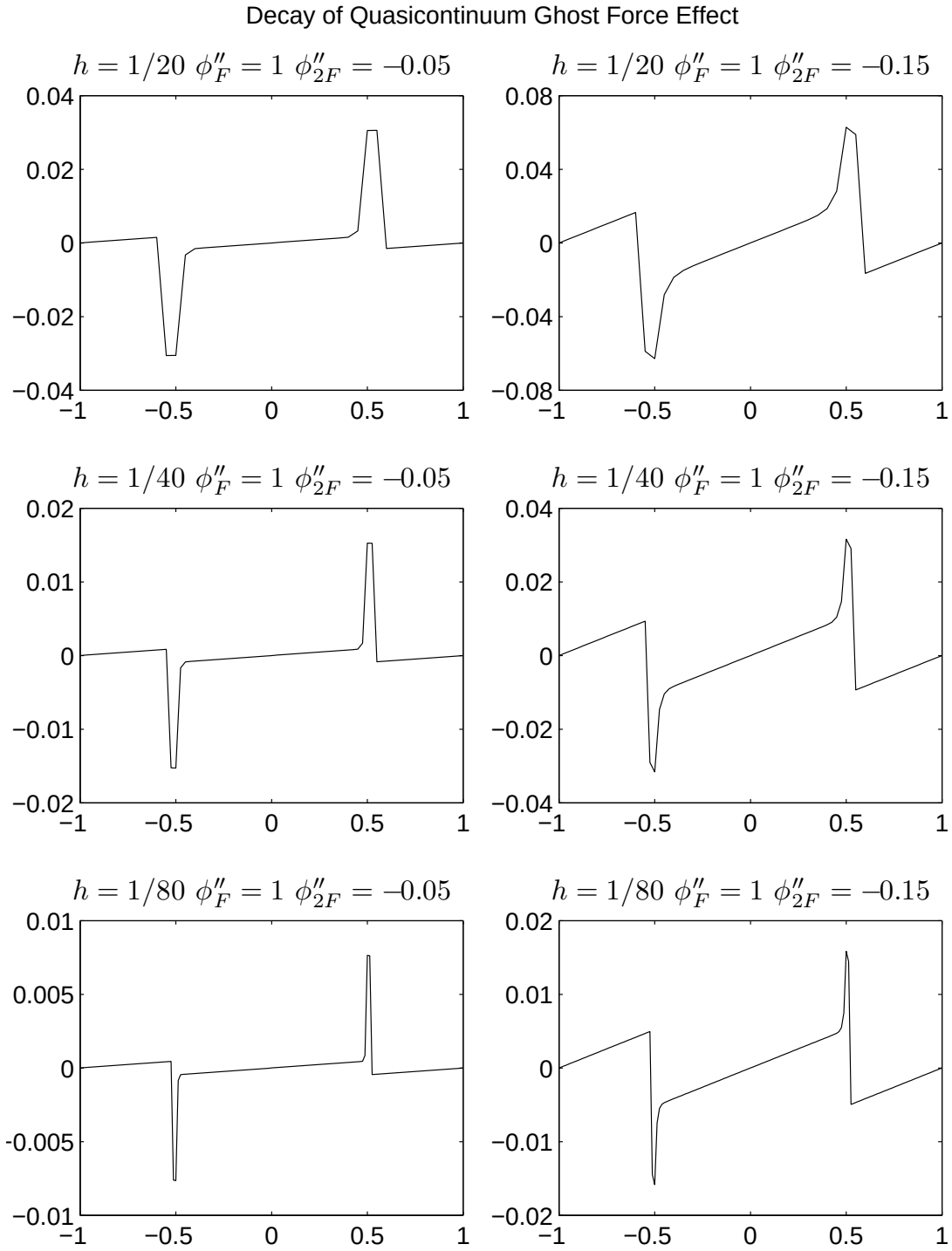

FIGURE 1. Error for the energy-based quasicontinuum approximation, $\mathbf{u}_{qc}$. We observe that the magnitude of the error is O(h). However, the oscillation near the interface means that the error in the displacement gradient is O(1) in the interfacial region. The average deformation gradient, F, for the right column is close to failing the stability condition $\phi''_F + 5\phi''_{2F} > 0$. In all plots $K = N/2$ and $\phi'_{2F} = 1$.

interface. Hence, the odd solution is given by

$$(\mathbf{u}_{qc})_j = \begin{cases} mhj + \beta\left(\frac{\lambda^j - \lambda^{-j}}{\lambda^K}\right), & 0 \le j \le K, \\ mhj - m + \tilde{u}_{K+1}, & j = K+1, \\ mhj - m, & K+2 \le j \le N, \end{cases} \tag{3.2}$$

where the coefficients $m, \tilde{u}_{K+1}$, and β can now be found by satisfying any three of the equations in the interface, $j = K-1, \dots, K+2$.

3.2. **Magnitude of the Solution.** We focus on the equations at $j = K-1, K+1$, and $K+2$ and split the interface equations as $(A_K + hB)\mathbf{x} = h\mathbf{b}$, where

$$A_K = \begin{bmatrix} \frac{1}{2}\phi''_{2F} & -\frac{1}{2}\phi''_{2F} & \phi''_{2F}\gamma_{K+1} - \frac{1}{2}\phi''_{2F}\gamma_{K-1} \\ -\phi''_F - \frac{5}{2}\phi''_{2F} & 2\phi''_F + \frac{13}{2}\phi''_{2F} & -\phi''_F\gamma_K - 2\phi''_{2F}\gamma_K - \frac{1}{2}\phi''_{2F}\gamma_{K-1} \\ -\frac{1}{2}\phi''_{2F} & -\phi''_F - 4\phi''_{2F} & -\frac{1}{2}\phi''_{2F}\gamma_K \end{bmatrix},$$

$$B = \begin{bmatrix} \phi''_{2F} & 0 & 0 \\ -\phi''_{2F} & 0 & 0 \\ \phi''_{2F} & 0 & 0 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} m \\ \tilde{u}_{K+1} \\ \beta \end{bmatrix}, \quad \mathbf{b} = \frac{1}{2}\phi'_{2F}\begin{bmatrix} -1 \\ 1 \\ -1 \end{bmatrix},$$

and $\gamma_j = \frac{\lambda^j - \lambda^{-j}}{\lambda^K}$. We note that A_K, B, and $\mathbf{b}$ do not depend on h directly, though A_K may have indirect dependence if K scales with h as in Figure 1. Therefore, we can neglect B and conclude that $\mathbf{x}$ is $O(h)$ provided that A_K^{-1} exists and is bounded uniformly in K.

Lemma 3.1. *For all K satisfying $2 \le K \le N-2$, the matrix A_K is nonsingular and $||A_K^{-1}|| \le C$ where $C > 0$ is independent of K.*

Proof. Applying row reductions gives the upper triangular form

$$\widetilde{A} = \begin{bmatrix} \frac{1}{2}\phi''_{2F} & -\frac{1}{2}\phi''_{2F} & \phi''_{2F}\gamma_{K+1} - \frac{1}{2}\phi''_{2F}\gamma_{K-1} \\ 0 & -\phi''_F - \frac{9}{2}\phi''_{2F} & \phi''_{2F}\gamma_{K+1} - \frac{1}{2}\phi''_{2F}\gamma_K - \frac{1}{2}\phi''_{2F}\gamma_{K-1} \\ 0 & 0 & \eta_K \end{bmatrix}$$

where

$$\eta_K = \left((\phi''_F)^2 + \tfrac{15}{2}\phi''_F\phi''_{2F} + \tfrac{53}{4}(\phi''_{2F})^2\right)(2\gamma_{K+1} - \gamma_K - \gamma_{K-1}) + \tfrac{1}{2}\phi''_{2F}\left(\phi''_F + \tfrac{9}{2}\phi''_{2F}\right)(\gamma_K - \gamma_{K-1}).$$

If the diagonal entries of $\widetilde{A}$ are non-zero, then A_K is nonsingular. The coercivity assumption $\phi''_F + 5\phi''_{2F} > 0$ (2.4) implies that $-\phi''_F - 9/2\phi''_{2F} < 0$ since $\phi''_{2F} < 0$, so the first and second diagonal entries are non-zero. Since the second term of η_K is negative, we can use the fact that $\gamma_K - \gamma_{K-1} < 2\gamma_{K+1} - \gamma_K - \gamma_{K-1}$ to see that

$$\begin{aligned} \eta_K &> \left((\phi''_F)^2 + 8\phi''_F\phi''_{2F} + \tfrac{62}{4}(\phi''_{2F})^2\right)(2\gamma_{K+1} - \gamma_K - \gamma_{K-1}) \\ &= \left(\phi''_F + \left(4 + \tfrac{1}{\sqrt{2}}\right)\phi''_{2F}\right)\left(\phi''_F + \left(4 - \tfrac{1}{\sqrt{2}}\right)\phi''_{2F}\right)(2\gamma_{K+1} - \gamma_K - \gamma_{K-1}) \\ &> 0. \end{aligned}$$

Therefore, A_K^{-1} exists for all K. Taking limits, we find

$$\lim_{K\to\infty} \eta_K \ge \left(\phi''_F + \left(4 + \tfrac{1}{\sqrt{2}}\right)\phi''_{2F}\right)\left(\phi''_F + \left(4 - \tfrac{1}{\sqrt{2}}\right)\phi''_{2F}\right)\left(2\lambda - 1 - \lambda^{-1}\right) > 0,$$

where we note that the elementary matrices corresponding to the row reduction operations did not depend on K so that $\lim_{K\to\infty} A_K$ is nonsingular. The inverse of a matrix is continuous as a function

of the entries whenever the matrix is nonsingular. Thus, the fact that $\lim_{K\to\infty} A_K$ is nonsingular implies that $\lim_{K\to\infty} ||A_K^{-1}||$ is finite. Since $||A_K^{-1}||$ is finite for all K and $\lim_{K\to\infty} ||A_K^{-1}||$ is finite, we conclude that $||A_K^{-1}||$ is uniformly bounded. □

Thus, we have that $m, \tilde{u}_{K+1}$, and β are all $\mathrm{O}(h)$. We can express the derivative, $\mathbf{u}'_{qc}$, as

$$(\mathbf{u}'_{qc})_j = \begin{cases} m + \frac{\beta}{h}\left(\frac{\lambda^{j+1}-\lambda^{-j-1}}{\lambda^K} - \frac{\lambda^j-\lambda^{-j}}{\lambda^K}\right), & 0 \le j \le K-1, \\ m - \frac{m}{h} + \frac{\tilde{u}_{K+1}}{h} - \frac{\beta}{h}\left(\frac{\lambda^K-\lambda^{-K}}{\lambda^K}\right), & j = K, \\ m - \frac{\tilde{u}_{K+1}}{h}, & j = K+1, \\ m, & K+2 \le j \le N-1, \end{cases}$$

where $u'_{-j-1} = u'_j$ for $j = 0, \ldots, N-1$.

Theorem 3.1. *Let $\mathbf{u}_{qc}$ be the solution to the QC error equation (2.15). Then for $1 \le p \le \infty$, $2 \le K \le N-2$, and h sufficiently small, the error can be bounded by*

$$||\mathbf{u}_{qc}||_{\ell_h^\infty} \le Ch,$$
$$||\mathbf{u}_{qc}||_{w_h^{1,p}} \le Ch^{1/p},$$

where $C > 0$ is independent of h, K, and p.

Proof. The result for the ℓ^∞ norm follows from the fact that all terms in (3.2) are $\mathrm{O}(h)$. To show the bound on $w^{1,p}$, we first apply the triangle inequality to separate the $m, \frac{\tilde{u}_{k+1}}{h}, \frac{m}{h}$, and $\frac{\beta}{h}$ terms which we bound using the fact that $\tilde{u}_{K+1}, m$, and β are $O(h)$. We have

$$\begin{aligned} ||\mathbf{u}_{qc}||_{w_h^{1,p}} &= ||\mathbf{u}_{qc}||_{\ell_h^p} + \left|\left|\mathbf{u}'_{qc}\right|\right|_{\ell_h^p} \\ &\le ||\mathbf{u}_{qc}||_{\ell_h^p} + |m| + \left(2\left|\frac{m}{h}\right|^p h\right)^{1/p} + \left(4\left|\frac{\tilde{u}_{K+1}}{h}\right|^p h\right)^{1/p} \\ &\quad + 2\left(h\sum_{j=-K}^{K}\left|\frac{\beta}{h}\frac{(\lambda^j-\lambda^{-j})}{\lambda^K}\right|^p\right)^{1/p} \\ &\le Ch^{1/p} + \frac{2|\beta|}{h}\left(2h\sum_{j=0}^{K}\left|\frac{\lambda^j}{\lambda^K}\right|^p\right)^{1/p} \\ &\le Ch^{1/p} + \frac{2|\beta|}{h}\left(2h\frac{\lambda^p}{\lambda^p-1}\right)^{1/p} \\ &\le Ch^{1/p}. \end{aligned}$$

□

Finally, we show that the pointwise error in the derivative, $\mathbf{u}'_{qc}$, decays exponentially in j to $\mathrm{O}(h)$ away from the interface in the atomistic region and decays immediately to $\mathrm{O}(h)$ away from the interface in the continuum region.

Lemma 3.2. *There is a $C > 0$ such that $|(\mathbf{u}'_{qc})_j| \le Ch$ for all $0 \le j \le K + \frac{\ln h}{\ln \lambda}$ and $K+2 \le j \le N$. Thus, the interface has size $O(h|\log h|)$.*

Proof. For h sufficiently small, we have that $\max(m, \beta) \le Ch$. Since $u'_j = m$ for $K+2 \le j \le N$, in this region $u'_j \le Ch$. For the terms $0 \le j \le K-1$ it is sufficient to show that the exponential term

is less than or equal to Ch. For $0 \leq j \leq K + \frac{\ln h}{\ln \lambda}$, we have that

$$\begin{aligned}\left(\frac{\lambda^{j+1} - \lambda^{-j-1}}{\lambda^K} - \frac{\lambda^j - \lambda^{-j}}{\lambda^K}\right) &\leq \lambda^{j+1-K} \\ &\leq \lambda^{K+\frac{\ln h}{\ln \lambda}+1-K} \\ &\leq Ch. \end{aligned}$$

□

Remark 3.1. In order reduce the degrees of freedom, the continuum region is coarsened in computations using the quasicontinuum method. For simplicity, coarsening was omitted from the model presented in this paper, but, in fact, the results are unchanged if it is used. Conventionally, coarsening only occurs away from the atomistic to continuum interface, so that no degrees of freedom are removed if they interact directly with the atomistic region. Since the solution u_j is linear for $K + 2 \leq j \leq N$, any level of coarsening produces an identical solution.

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